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Jacob Spendelow preps a reference electrode setup connected to a fuel cell enclosed in hardware. The setup measures electric potential at nine different points on the cathode and can gauge impurities as well as potential degradation affecting its performance.

Photo by Richard Robinson, XIT-TSS

Jacob Spendelow

Aiming for fuel cell durability through atomic-level control

by Kris Fronzak, ADEPS Communications

“Designing fuel cell electrodes is often described as a black art, not a science,” said Jacob Spendelow, a chemical engineer in Materials Synthesis and Integrated Devices, MPA-11. “A lot of it is just trial and error. We want to make better fuel cells, but that starts with understanding the fundamental stuff.”

By converting the chemical energy of a reaction between hydrogen and oxygen to electricity, fuel cells can power everything from light bulbs to submarines. Their main byproduct is water, making fuel cells a clean, compelling alternative to traditional gasoline-powered, combustion engine cars.

For Spendelow, who grew up in an “ultra-green” household and who always wanted to be a researcher, Los Alamos National Laboratory was an obvious pick after he graduated from the University of Illinois with his PhD in chemical engineering. “[MPA-11] is a really prominent group in the fuel

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“
A lot of people haven't achieved this [durability], over the years. It's a challenge, no question, but I wouldn't be working on it if I didn't think we had a chance.”



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I believe the refresh is an opportunity for MPA, especially when mindful that a notable strength of our Laboratory is the ability to integrate expertise across organizational boundaries.

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From Rick's desk

As most of you know, the LDRD program recently completed its first refresh in nearly a decade. Some are skeptical about the changes and remain concerned about how these changes may impact their research. As such, I thought I would focus this article on the changes to LANL's LDRD program and its impact to MPA.

The refresh was motivated by several goals, including a desire to more effectively integrate science into LANL's mission and the need to ensure that our mission rests on a strong science foundation to productively address long-standing challenges. I believe the refresh is an opportunity for MPA, especially when mindful that a notable strength of our Laboratory is the ability to integrate expertise across organizational boundaries. LDRD provides a fantastic mechanism to develop collaborations and successfully address key scientific challenges while establishing new capabilities and relationships. At its core, LDRD will continue to contribute to several goals including building on our science and engineering reputation, developing new approaches to address key national security challenges, and enhancing critical skills for long-term mission objectives.

The refresh resulted in a minor shift to the overall balance and structure of the program. A new LDRD category, Mission Foundations, was developed. For FY17 this category is relatively small in terms of budget. Funded projects in this category will have a duration of only two years. The underlying objective of this category is to enable technology maturation, which may include prototype demonstrations for known mission needs. A goal for funded projects in this category is to transition to programmatic funding although this is not a requirement. This provides an outstanding opportunity for MPA to transition our foundational science to applied programs. Going forward the Science Advisory Panel will rely more on the guidance provided in the Laboratory's Strategic Investment Plan, and the Strategy Committee will remain mindful of LANL's overall mission when assessing LDRD proposals.

With change comes opportunity, so some may question the impact of the LDRD refresh relative to MPA's overall budget. From FY16 our total LDRD budget has increased by 6%. In FY17, ADEPS endorsed 7 Early Career proposals and MPA received funding for 1 of the 10 from across the institution. In the category of Mission Foundations, 8 proposals were funded across LANL, 2 of which are led by MPA. Of the 14 new starts in Directed Research, 2 are led by MPA, and finally, of the 40 new ER projects, MPA is leading 7. In summary, MPA's LDRD portfolio for FY17 remains as strong as ever, despite the Laboratory-wide decrease in LDRD funding.

The changes to the LDRD program are notable—while the value of LDRD remains as strong as ever. Our ability to successfully respond quickly to the new call in the Mission Foundation category is an example of our agility and willingness to embrace new opportunities during times of change. We will continue to monitor the health and science of our LDRD program. It is an interesting time of transition for LANL; with that comes change and opportunity. I remain extremely proud of the science performed in MPA and look forward to new opportunities to engage with scientists and engineers in other areas of LANL's mission to further strengthen our portfolio.

MPA Deputy Division Leader Rick Martineau



From Mike's desk

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The reviewers determined our MS&E projects to be of consistently high quality and that our personnel are viewed as having significant leadership positions in important areas of materials research.

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Mike

The DOE Office of Basic Energy Sciences (BES) Materials Science and Engineering (MS&E) program continues to be a crucial source of funding for LANL's fundamental materials research efforts and is of particular importance to MPA's research portfolio. BES funds the Center for Integrated Nanotechnologies, our joint LANL-Sandia National Laboratories user facility focusing on nanoscale materials research. BES also funds seven individual field work proposals (FWPs) that involve teams in four LANL divisions (MPA, MST, T, and NSEC). These seven projects were the focus of an on-site review conducted at LANL on November 2-3, 2016. MPA is home to three MS&E projects involving functionality that is derived from electronic and magnetic degrees of freedom. Leonardo Civale is the PI for a project titled "Towards a universal description of vortex matter in superconductors" that focuses on vortex dynamics across a broad spectrum of superconductors. Neil Harrison leads the "Science at 100 tesla" project that utilizes the 100 tesla magnet at the National High Magnetic Field Facility-Pulsed Field Facility to study correlated electron phenomena in superconductors, Dirac materials, and topological systems. Filip Ronning leads our long-standing "Complex electronic materials" project that studies emergent quantum states in complex materials through an approach that closely couples materials discovery with relevant spectroscopy and wide-ranging characterization activities. MST researchers lead two MS&E projects that focus on materials functionality derived from structure. Carlos Tome is PI on "Dilatational and shear transformations in HCP metals: interfacial defects and collective interactions," while Blas Uberuaga leads a project involving "Disorder and diffusion in complex oxides: prediction and control." The remaining two projects are funded through the MS&E theoretical condensed matter physics program office; they are led by NSEC's Sasha Balatsky ("Integrated modeling of novel and Dirac materials") and T Division's Art Voter ("Accelerated molecular dynamics methods").

The on-site review panel that convened in November was tasked with examining the research progress and accomplishments of our seven MS&E projects during the prior three fiscal years (FY14-16) as well as the proposed research plans for the next three years (FY17-19). The reviewers were asked to consider the scientific and technical merit of each BES project, the appropriateness of the proposed technical approach, competence of the personnel involved, adequacy of both resources and budget to carry out the technical work, synergy and interactions between the PIs and their project teams, and utilization of LANL's unique facilities.

The reviewers determined our MS&E projects to be of consistently high quality and that our personnel are viewed as having significant leadership positions in important areas of materials research. They were also laudatory regarding our use of LANL's unique facilities and the high competency exhibited by all the project co-investigators. Overall, BES concludes that the LANL MS&E program demonstrates a strong research portfolio. This very positive outcome is a testament to the efforts of the above-mentioned FWP PIs, their teams, and the program leadership provided by Don Rej and Toni Taylor.

Moving forward, we anticipate that BES will publish a call in the next year that will fund a new round of Energy Frontier Research Centers that would likely commence in the later part of FY18. Staff interested in this and other potential BES funding opportunity are encouraged to carefully examine BES's 2015 strategic document "Challenges at the frontiers of matter and energy: transformative opportunities for discovery science" and the just recently published report of the BES Basic Research Needs workshop on quantum materials for energy relevant technology. Both reports are available for download from the DOE BES website. Uncertainty prevails in Washington, but there may be opportunities that well-informed and properly prepared research can be utilized to strengthen LANL's fundamental materials research portfolio.

MPA-CMMS Group Leader Mike Hundley

Spendelow cont.

cell community. The modern fuel cell was basically invented here,” Spendelow said, referring to a 1990’s Lab discovery that cut by about 95% a fuel cell’s need for platinum, a costly precious metal, while concurrently boosting performance.

Following his conversion from postdoctoral researcher to Laboratory staff, Spendelow collaborated with researchers from MPA-11 and the National Institute of Standards and Technology on neutron radiography studies of water distribution in operating polymer electrolyte membrane fuel cells (PEMFCs). A change-of-station assignment brought him to the Department of Energy’s (DOE’s) Fuel Cell Technologies Office in Washington, D.C., where he advised on fuel cell science, analyzed fuel cells and related technologies, and supported development of fuel cell technology.

The position required that he stay abreast of the entire fuel cell field—knowledge that proved essential when he returned to MPA and Los Alamos in 2015. Spendelow is the Lab’s representative on the US DRIVE Fuel Cell Tech Team (FCTT), which includes representatives from automotive companies, laboratories, and the government, all of whom help the DOE with issues ranging from technical target setting for fuel cells to identifying and evaluating R&D needs.

As part of the MPA-11 Fuel Cell team, Spendelow collaborates with MPA researchers in fuel cell diagnostics and electrode design—research that supports the Laboratory’s Energy Security mission and its Materials for the Future science pillar.

He is also principal investigator on a newly launched project in PEMFC catalyst development. The DOE-funded “Electro-

catalysts Through Crystallography” undertaking includes his co-principal investigator and MPA-11 colleague Yu Seung Kim and researchers from Brown University, the University of Pennsylvania, University at Buffalo, and the private company EWII Fuel Cells.

In addition to cost, another hurdle to commercial fuel cell adoption is catalyst durability, which is hindered by the corrosive operating conditions. While PEM fuel cells are deployed in demonstration vehicles and are beginning limited commercialization, they still fall short of DOE targets for this technology, which are required for widespread consumer acceptance. The DOE has asked that the catalysts remain viable for 5,000-8,000 hours of operation—about the lifetime of a vehicle itself—and that they be tested in situ.

To produce catalysts that are both durable and more active than those to date, the team is using crystallographic techniques to produce a platinum alloy where the nanoparticles are fully ordered—that is, the atoms are deposited in certain positions in the overall structure. The team theorizes these ordered alloys will be more durable and more active than randomized alloys—where the atoms are disordered—which are more commonly employed in fuel cells.

“This idea is different from anything anyone else is doing out there, and worth pursuing,” said MPA-11 Group Leader Andrew Dattelbaum. “We need to test out some of these nanoparticles in more realistic environments.”

“A lot of people haven’t achieved this [durability], over the years. It’s a challenge, no question, but I wouldn’t be working on it if I didn’t think we had a chance,” said Spendelow.

Jacob Spendelow’s favorite experiment

What: Demonstrated that carbon monoxide electrooxidation on the (111) surface of platinum primarily takes place at defect sites.

Why: Carbon monoxide electrooxidation is an important reaction in fuel cells, and it’s also a “model system” used to better understand the electrochemical properties of catalysts like platinum.

When: 2005

Who: Jacob Spendelow, Jason Goodpaster, Paul Kenis, Andrzej Wieckowski (all at University of Illinois at the time)

How: We studied carbon monoxide oxidation and the effect of surface structure using a variety of electrochemical and imaging techniques, and much of the data suggested that defects were the primary active sites for carbon monoxide oxidation, but it was difficult to rule out other factors.

The “a-ha” moment: We tried a variety of techniques to remove defects without success. But then we deposited a very small amount of silver on the platinum surface, and saw features associated with defects suddenly disappear while the rest of the surface remained unchanged. When we tried oxidizing carbon monoxide on the surface, we saw that the rate of oxidation was 25 times lower than normal, finally confirming that it had been the defect sites that were primarily responsible for carbon monoxide electrooxidation.

MPA staff in the news

Aiping Chen leads nanocomposite symposium organization

Aiping Chen (Center for Integrated Nanotechnologies, MPA-CINT) recently served as a leading symposium organizer for The American Ceramic Society's Electronic Materials and Applications 2017 (EMA 2017) conference.



Chen collaborated with other organizers to develop a session on multifunctional nanocomposites, in particular, highlighting recent advances in the growth, characterization, design, property prediction, and study of functional properties/device applications in oxide thin films and their nanocomposites. The symposium focused on the theoretical understanding, design, and prediction of material properties using first principles based methods; synthesis of oxide thin films, multilayers and vertically aligned nanocomposites; structure, defect, and interface characterization and their relationship to material properties; and device fabrication and integration strategies with existing technologies for energy harvesting, memories, actuators, sensors, and optical, electronic, and optoelectronic applications.

Chen, a member of the CINT nanoscale electronics and mechanics science thrust, received his PhD in electrical engineering from Texas A&M University. His research focuses on synthesizing complex oxide thin films and their nanocomposites, controlling functionalities via microstructure, defect and interface engineering, and exploring nanomaterial applications in nanoelectronics.

EMA 2017, held recently in Orlando, Florida, is The American Ceramic Society's annual meeting on advances and challenges in the field of electronic materials. It is designed to help researchers foster collaboration and exchange ideas in electroceramic materials and their applications in electronic, electromechanical, magnetic, dielectric and optical components, devices, and systems. Other symposium organizers were James Rondinelli (Northwestern University), Junwoo Son (Pohang University of Science and Technology, South Korea), Judith L. MacManus-Driscoll (University of Cambridge, United Kingdom), and Roman Engel-Herbert (The Pennsylvania State University).

CINT is a DOE Office of Basic Energy Sciences user facility jointly operated by Los Alamos and Sandia national laboratories.

Technical contact: Aiping Chen

Jennifer Hollingsworth named a 2016 Laboratory Fellow

Jennifer Hollingsworth (Center for Integrated, MPA-CINT) has been named a 2016 Los Alamos National Laboratory Fellow.



The Los Alamos Fellows organization, established in 1981, includes technical staff members who have been appointed by the Laboratory Director in recognition of their outstanding contributions and exceptional promise for continued professional achievement.

Hollingsworth is a nanomaterials and inorganic chemist at CINT. She and her team focus on the development of functional heterostructured nanomaterials possessing unique light-emission properties. Synthesized using low-temperature solution-phase chemistry techniques, the colloidal nanostructures have potential applications ranging from next-generation efficient lighting to nanomedicine. Hollingsworth's breakthrough discovery of "giant" QDs (gQDs) eliminated for the first time the problematic photophysical phenomenon of "blinking" (interruptions in light emission that represent a significant drawback for standard QDs).

Her work spans the design and elucidation of nanocrystals intentionally engineered for new functionality and the development of novel synthetic methods. She finds great satisfaction in knowing that gQDs developed in her laboratory are enabling the experiments of researchers across the globe through the CINT User Program. She also delights in her interactions with students and postdocs, mentoring more than 30, many of whom have pursued independent research careers in national labs, academia, and industry. Hollingsworth received the Los Alamos Fellows Prize in 2013 and is councilor for the American Chemical Society Colloid and Surface Science Division.

Scott Crooker (Condensed Matter and Magnet Science, MPA-CMMS) (see below), Dean Preston (Materials and Physical Data, XCP-5) and Roger Wiens (Space and Remote Sensing, ISR-2) were also named Fellows.

Laboratory Director Charlie McMillan lauded the 2016 honorees, whose scientific accomplishments "not only show the breadth of our multidisciplinary scientific and technical capabilities, but also embody the spirit and character of our Laboratory and its essential role in solving our nation's most important challenges." Fellows are limited to 2% of the Laboratory's technical staff. They advise management

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Staff cont.

on important issues, promote scientific achievement, and organize symposia and public lectures.

Technical contact: Jennifer Hollingsworth

Scott Crooker recognized for scientific achievements, contributions

Scott Crooker (Condensed Matter and Magnet Science, MPA-CMMS) has been recognized as a 2016 American Association for the Advancement of Science (AAAS) Fellow and a 2016 Los Alamos National Laboratory Fellow. The condensed-matter physicist and optical spectroscopist at the National High Magnetic Field Laboratory-Pulsed Field Facility (NHMFL-PFF) was also recently selected as a 2017 American Physical Society (APS) Outstanding Referee.



AAAS Fellowship is awarded to AAAS members by their peers in recognition of scientifically or socially distinguished efforts to advance science or its applications. Crooker was chosen for distinguished contributions to condensed matter physics, particularly in the development of magneto-optical spectroscopies and their application to fundamental properties of novel semiconductor materials. The AAAS is the world's largest general scientific society and publisher of the journal *Science*. This year, AAAS awarded fellowship to 391 members, including Bill Louis (Subatomic Physics, P-25).

"The AAAS fellowship is an honor that recognizes Scott's and Bill's scientific achievements and leadership," said Carol Burns, deputy principal associate director for Science, Technology and Engineering. "Their work helps Los Alamos succeed in its national security mission and has an international impact."

The Los Alamos Fellows organization, established in 1981, annually recognizes technical staff members who have made sustained outstanding contributions and exceptional promise for continued professional achievement.

Peter B. Littlewood, director of Argonne National Laboratory, said Crooker is "consistently the most stimulating researcher in the field of semiconductor optics I know."

Crooker's selection as an Outstanding Referee was based on his work assessing manuscripts for publication in the APS's *Physical Review* journals. Award selection is based on the quality, number, and timeliness of the reports, without

regard for APS membership, country of origin, or field of research.

Crooker, who received a PhD in physics from the University of California, Santa Barbara, joined Los Alamos in 1998 as a Director's Postdoctoral Fellow at the NHMFL-PFF. Since 2000, he has been a staff scientist. He and his team develop magneto-optical techniques to study the dynamic behavior of electron spins and magnetic moments in novel semiconductor materials. His contributions include designing experiments to image spin-polarized currents in semiconductors, developing and applying optical spectroscopies to probe spin and magnetization fluctuations, and studying spin dynamics in condensed matter. He won the 2007 Los Alamos Fellows Prize for Research and is also a fellow of the APS and Optical Society of America. Crooker has served as a divisional associate editor for *Physical Review Letters* and has supervised about 30 students and postdoctoral researchers.

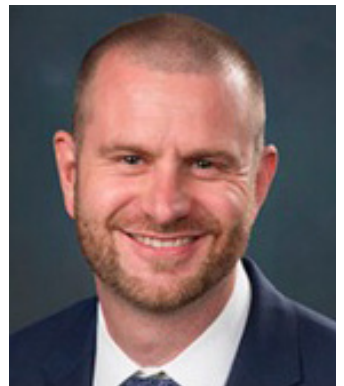
Technical contact: Scott Crooker

Marc Janoschek, Jennifer Martinez, Jian-Xin Zhu receive 2016 Fellows Prize in science and engineering

Marc Janoschek (Condensed Matter and Magnet Science, MPA-CMMS), Jennifer Martinez (Center for Integrated Nanotechnologies, MPA-CINT), and CINT theory and simulation of nanoscale phenomena co-thrust leader Jian-Xin Zhu (Physics of Condensed Matter and Complex Systems, T-4) are recipients of the Laboratory Fellows Prize in science and engineering. The award commends individuals for outstanding research performed

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**Clockwise from top right:
Marc Janoschek, Jian-Xin
Zhu, Jennifer Martinez**



Staff cont.

at the Laboratory that was published within the last 10 years and has had a significant impact on its discipline or program.

Janoschek led the first experiment to detect a fluctuating magnetic state in plutonium by assembling a multidisciplinary team that utilized plutonium-242 to carry out measurements at the Spallation Neutron Source; many have said this is the most significant measurement on plutonium in a generation. His research focuses on the use of elastic and inelastic neutron scattering to elucidate complex behavior in materials exhibiting emergent phenomena. This important work supports the programmatic efforts of the Lab and helps Los Alamos maintain its position as the recognized leader in actinide science and correlated electron materials research.

Martinez is among the best-known nanocluster scientists in the world. Her research has focused on the development of biosensors for threat reduction, tuberculosis, and breast cancer as well as the synthesis and characterization of optical and biologically reactive polymers. The nanocluster research has demonstrated the ability to control the synthesis and tailoring of the photophysical properties of small metal nanoclusters, which represents an emerging and interesting class of materials that can be used in to create new biological detectors that overcome many difficulties of earlier approaches.

Zhu broadly impacted actinide science and nanotechnology work at the Lab by upending the conventional picture of when the transition to strong correlations occurs in delta and alpha plutonium. His research focuses on the development and application of quantum, many-body, first-principles electronic structure theory to strongly correlated electronic materials. Zhu's work on plutonium is an achievement in computational and theoretical physics that represents a dramatic leap forward; it has attracted a great deal of attention in the field of correlated electron systems.

Christopher Stanek (Materials Science in Radiation and Dynamics Extremes, MST-8) and Dana Dattelbaum (Explosive Science and Shock Physics, M-DO) received the Fellows Prize in leadership.

"These scientists are being recognized for mission-relevant research and leadership that maintain the Lab's long-standing reputation for innovative scientific discoveries," said Chuck Farrar, the Engineering Institute Leader at the Laboratory's National Security Education Center and the coordinator of the Fellows Organization. "I congratulate all of them on their achievements."

Technical contacts: Marc Janoschek, Jennifer Martinez, Jian-Xin Zhu

Jinkyong Yoo presents invited seminar on 2D/3D van der Waals heterostructures

Jinkyong Yoo (Center for Integrated Nanotechnologies, MPA-CINT) recently gave an invited special seminar at the University of California, San Diego on "2D/3D van der Waals heterostructures: Nucleation and Characteristics."



Yoo focused on combining conventional three-dimensional (3D) materials and atomically thin two-dimensional (2D) materials such as graphene, hexagonal boron nitride, and transition metal dichalcogenides emergent in nanoscience. He discussed ways to control nucleation of three-dimensional (3D) materials on those 2D layers, dramatic changes of electrical properties of both 2D and 3D materials in the same heterostructures, and related them to flexible devices, which are of interest due to the potential of strain-free and crystalline 3D materials on atomically thin 2D materials.

Yoo, who earned his PhD in materials science and engineering from Pohang University of Science and Technology in South Korea, is a member of CINT's nanoelectronics and mechanics thrust. At CINT, he studies the preparation of semiconductor heterostructures, such as nanowires and thin films, in nanoscales/microscales via chemical vapor deposition. He also performs research of devices based on the synthesized semiconductor heterostructures.

Prior to joining the Lab, Yoo researched wide band gap semiconductor heterostructures (III-nitrides and II-oxides) for photonic devices, such as light-emitting devices and microcavities for polaritonics.

Yoo's work supports the Laboratory's Energy Security mission and its Materials for the Future science pillar by tailoring materials to perform beyond their basic properties, thereby enabling controlled functionality, a central vision of the Laboratory's materials strategy. CINT is a DOE Office of Basic Energy Sciences User Facility, operated jointly by Los Alamos and Sandia national laboratories.

Technical contact: Jinkyong Yoo

Fulfilling the promise of quantum materials through research using high magnetic fields

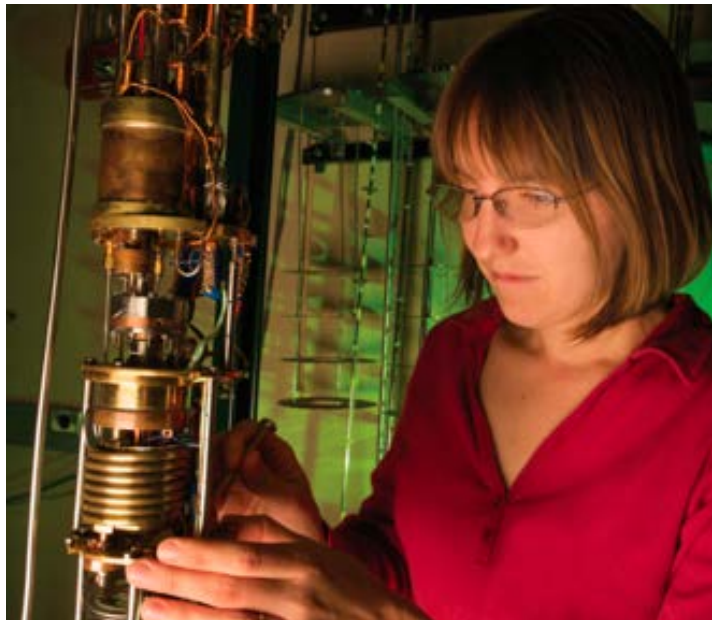
Quantum materials are an intriguing and growing field of scientific study due to the rich functionalities enabled by their emergent phenomena. By probing the complex behaviors arising from the material's unique collective physical, chemical, and biological response, researchers are presented with the possibility of exploiting these properties for technological devices designed to address some of the most challenging energy security challenges.

To probe quantum materials and their emergent phenomena, high magnetic fields are critical, said Vivien Zapf, a physicist at Los Alamos National Laboratory's National High Magnetic Field Laboratory-Pulsed Field Facility (NHMFL-PFF). "High magnetic fields offer a powerful and exquisitely versatile tool for probing the fundamental properties that lie at the heart of this exciting class of materials, which includes metals, superconductors, semiconductors, and magnetic insulators."

"For example, for the past ten years users of the magnet lab have been exploiting our unique capabilities to unravel the properties of topological materials, which is the subject of this year's Nobel Prize," she said. "Yet existing technology can only take us so far."

During a talk to the National Science Foundation, as part of the NHMFL's site review, Zapf made a case for higher magnetic fields and advanced tools by identifying opportunities in quantum materials science and the challenges faced. These materials, through which a better understanding of their fundamental properties offers great potential, include the following.

- **Superconductors:** The grand challenge of understanding high-temperature superconductivity is now closer than ever before with proposed new magnet developments that will further allow researchers to chart the Fermi surface of unconventional superconductors and to better understand the quantum critical phenomena that lie at the heart of superconductivity.
- **2D semiconductors:** Historically, experiments in magnetic fields have played a central role in elucidating the electronic and optical properties of semiconductors. In the new generation of atomically thin semiconductors like graphene and MoS_2 , very large magnetic fields (> 50 tesla) are particularly important due to the large electron masses and extremely large electron-hole binding energies in these materials that arise from the two-dimensional nature of the excitons. These materials have promising applications for optoelectronics and flexible transparent and biocompatible electronics.
- **Topological materials:** as noted, topology in condensed-matter physics promises new routes to discrete and protected states and it is the topic of this year's Nobel Prize in Physics. Critically important information about topological band structures and magnetic states can be uncovered with high magnetic fields.



Vivien Zapf, a physicist at the NHMFL's Pulsed Field Facility at Los Alamos National Laboratory, studies quantum magnetism and magnetoelectric materials. The facility is behind much of the Laboratory's quantum materials science, including topology and research into high-temperature superconductivity.

- **Multifunctional magnets:** The new generation of multifunctional devices relies on complex magnetic spin structures, the properties of which can be unraveled by combining neutron scattering and physical properties measurements in high magnetic fields. Higher temperature functional materials require higher magnetic fields to compete with the intrinsic interactions within the materials.

During a talk to the National Science Foundation, as part of the NHMFL's site review, Zapf made a case for higher magnetic fields and advanced tools by identifying opportunities in quantum materials science and the challenges faced.

Los Alamos's Pulsed Field Facility is a part of the NHMFL, a national user facility funded by the National Science Foundation and the State of Florida. With a broad range of capabilities across its facilities in Los Alamos, Florida State University, and the University of Florida, it is the largest and highest-powered magnet laboratory in the world. The NHMFL provides users access to expertise and tools found nowhere else, allowing them to perform innovative and pioneering studies in materials, biology, medicine, environmental, and energy research. The NHMFL-PFF supports the Laboratory's National Security Science mission and Materials for the Future science pillar and contributes to the Science of Signatures and Integrating Information, Science, and Technology for Prediction science pillars. For more about the capabilities of the NHMFL-PFF, please see nhmfl.lanl.gov.

Technical contact: Vivien Zapf

Metasurfaces transitioning to applications

Metamaterials are artificially engineered media that have allowed the demonstration of many exotic electromagnetic phenomena, including negative refractive index, electromagnetic cloaking, and super-resolution lenses to name a few. While bulk metamaterials pose severe fabrication challenges, planar metamaterial architectures—metasurfaces—offer alternative avenues to accomplish desirable functionalities. Metasurfaces allow independent control of the amplitude, phase, polarization, and propagation of electromagnetic waves through tailoring the design parameters of the constituent subwavelength resonators. Particularly, metasurfaces containing few layers of specially designed resonator arrays have shown unprecedented capability in manipulating electromagnetic waves, enabling unique electromagnetic phenomena including anomalous refraction/reflection, near-unity absorption, polarization conversion, flat lensing, and electromagnetic phase-shifting.

The metamaterial group at the Center for Integrated Nanotechnologies (MPA-CINT) has made groundbreaking contributions in developing new concepts and demonstrating novel metasurfaces for applications in the technically challenging terahertz regime. Recently, the group expanded the breadth of metasurface research in the domains of the electromagnetic spectrum, including visible and microwave frequencies, for practical applications.

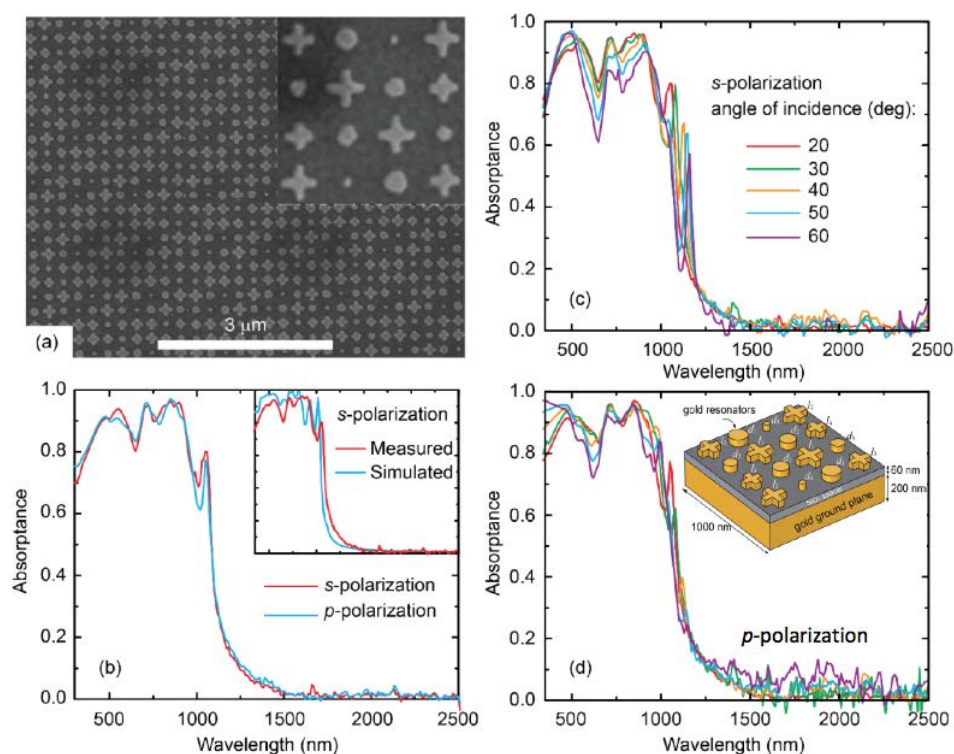
For example, rationale-designed metasurfaces will allow high absorption in the entire solar spectrum but emission only at a narrow spectral window matching the bandgap of photovoltaic materials. This unique property can be applied

to an intermediate photon-management system to dramatically enhance the efficiency of solar thermo-photovoltaics (STPV). Recently, the group has made important progress in this direction by demonstrating an ultra-thin metasurface with the unit cell consisting of eight pairs of gold nanoresonators separated from a gold ground plane by a thin silicon dioxide spacer (see Fig. 1). It was shown that the metasurface can function as a polarization independent, omnidirectional, and broadband solar absorber, with greater than 90% absorption in the visible and near-infrared wavelength range, and exhibiting low absorptivity (emissivity) at mid- and far-infrared wavelengths, the desirable properties to be used in STPV.

As a second example, the metamaterial group has demonstrated a metasurface-based ultrathin flat lens antenna operating at microwave frequencies. The metasurface lens antenna is composed of three thin layers of metallic structures: an array of subwavelength resonators sandwiched by two orthogonal gratings with 5-mm inter-layered air spacing (see Fig. 2), providing a parabolic phase distribution in the radial direction to function as a lens antenna. It demonstrated excellent focusing/collimating of broadband microwaves from 7.0-10.0 GHz, with an absolute gain enhancement of 18 dBi at the central wavelength of 9.0 GHz. The high-performance beam collimation was evidenced by the small 3dB directionality angle $< 4.5^\circ$. The demonstrated metasurface lens antenna will enable high gain, broadband, lightweight, low-cost, and easily deployable

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Figure 1 (a) SEM image of a portion of the fabricated absorber. The inset shows an expanded view of the super-cell. (b) Experimentally measured extinction for s - and p - polarizations at 20° angle of incidence, and at various angles of incidence for s - (c) and p -polarized (d) light. Inset to (b) is a comparison between experiments and simulations both at 20° angle of incidence for s -polarized incident light. Inset to (d) shows the schematic design of the super-cell.



Metasurfaces cont.

flat transceivers for microwave communication, overcoming the severe limitations of conventionally used parabolic reflectors and dielectrics lenses for beam collimation or focusing.

The research benefited from the fabrication and characterization capabilities in the Center for Integrated Nanotechnologies (CINT), a DOE Office of Science national user facility. The research, funded in part by the Lab's LDRD program, is relevant to the Laboratory's national security mission. The innovations of this research address the key science issues encountered in the development of future photonic technologies, energy harvesting, and lightweight communication devices.

Researchers include Abul Azad, Anatoly Efimov, and Hou-Tong Chen (MPA-CINT); Diego Dalvit and Wilton Kort-Kamp (Physics of Condensed Matter and Complex System, T-4); Milan Sykora (Inorganic Isotope and Actinide Chemistry, C-IIAC); Antoinette J. Taylor (Chemistry, Life and Earth Sciences, ADCLES); and Nina Weisse-Bernstein (Space and Remote Sensing, ISR-2). Reference: "Metasurface Broadband Solar Absorber," *Scientific Reports*, **6**, 20347(2016).

Technical contact: Abul Azad

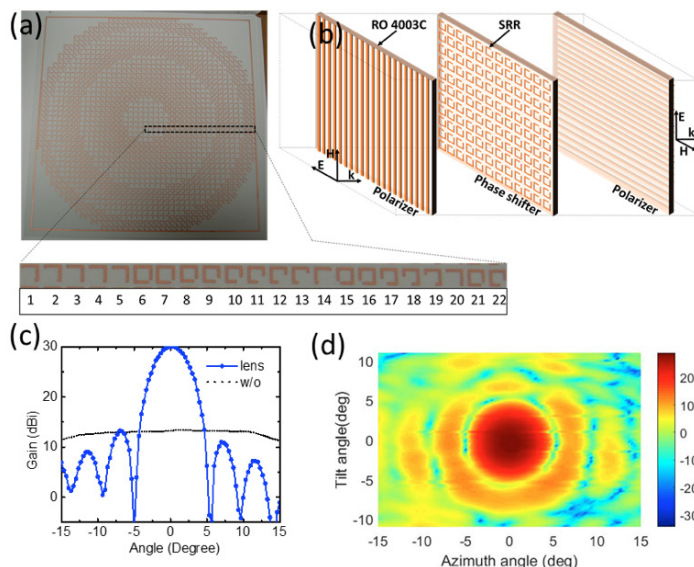


Figure 2) Design and characterization of the microwave metasurface flat lens. (a) Optical image of the fabricated metasurface layer that provides the required phase distribution for focusing the microwave beam. Inset shows radial metallic resonators from center to edge. (b) Schematics of the lens layers. (c) Measured far field gain of the flat lens antenna while fed by a horn antenna (blue) and the gain of a horn antenna without the lens (black). (d) Measured beam profile at the focus showing a dominant main lobe.

Annual CINT users meeting celebrates 10 years of innovation

The Center for Integrated Nanotechnologies' (CINT) 16th Annual Users Meeting, held recently in Santa Fe, highlighted 10 years of innovation at the national user facility, drawing more than 200 participants from 5 industries, 10 government agencies and laboratories, and 36 national and international universities.

The two-day meeting kicked off with three plenary presentations. Dmitri Basov (University of California, San Diego) spoke on "Quantum Materials: Insights from Infrared Nano-optics;" Thomas Mallouk (Pennsylvania State University) presented on "Assembly and Disassembly of Layered Solids;" and Juan de Pablo (University of Chicago) discussed "Nanoparticles in Liquid Crystals, and Liquid Crystals in Nanoparticles."

Three symposia also took place during the meeting. "Quantum Materials Integration" was organized by Michael Lilly (CINT-Sandia National Laboratories, CINT-SNL) and Han Htoon (MPA-CINT). It focused on research efforts in initializing, measuring, and manipulating quantum states in spin and photonics systems. Sang Bok Lee (University of Maryland) and Katherine Jungjohann (CINT-SNL) organized the symposium "Electrochemical Nanostructures: Mesoscale Architectures and Integration," which focused on progress and future perspectives in the science of electrochemical nanostructures. "From Molecules to Integrated Structures—Assembly



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and Fabrication across Length Scale," examined approaches to controlling structure and function to create functional soft materials. It was organized by Millie Firestone (MPA-CINT) and Dale Huber (CINT-SNL).

The user meeting also included a poster session featuring research by 50 users and CINT scientists; an evening event celebrating CINT's 10-year anniversary, with talks by former and current members of the CINT management team; and a meeting of the User Executive Committee. The 2017 Users meeting was followed by "The Materials Science and Data Technology Nexus" workshop, organized by CINT nanoscale electronics and mechanics co-thrust lead Nate Mara (MPA-CINT).

CINT is a DOE Office of Basic Energy Sciences user facility jointly operated by Los Alamos and Sandia national laboratories.

Technical contact: Alex Lacerda

LANL prototype proves design concepts for plutonium electromagnetic isotope separator

Los Alamos researchers in collaboration with external colleagues have successfully developed and tested a high-throughput electromagnetic isotope separator (EMIS) capable of producing gram-scale quantities of high purity isotopes in a single day. Among others, they have successfully created indium-113 with 99.9975% purity in a single pass and exceeded the researchers' expectations for resolution and separation quality. The primary purpose of this EMIS is to serve as a prototype for ion source and instrument modifications to mitigate risks associated with a similar instrument that will be used to isotopically refine the nation's plutonium-242 (Pu-242) inventory.

Plutonium-242 is an isotope of plutonium chemically identical to but approximately 16 times less radioactive than the fissile isotope plutonium-239, which is the isotope used in the primaries of nuclear weapons. Concerns surrounding nuclear criticality and nuclear weapons proliferation are significantly reduced with plutonium-242, which makes it an ideal resource for accelerating much of the plutonium science and engineering mission of the Laboratory. This can be accomplished by enabling the strategic use of lower hazard/security category radiological facilities and by bringing a broader suite of technical capabilities, personnel, and instrumentation to bear on plutonium-related problems.

The isotopic purity of the existing plutonium-242 inventory is quite attractive ($\geq 90\%$), but it is contaminated with enough other highly radioactive isotopes (e.g. americium-241 and plutonium-238) that using it in its current form is dubious. As such, refining the inventory to a plutonium-242 content of 99.9+% would allow researchers to use up to 600 g in existing radiological facilities. Given the performance and throughput realized by the prototype instrument, achieving the necessary purity levels is within reach. The team intends to complete the design of a plutonium separator within a year, and to manufacture a dedicated plutonium machine about a year after that.

Celebrating service

Congratulations to the following MPA Division employees celebrating service anniversaries recently:

David Reagor, MPA-11	30 years
Roman Movshovich, MPA-CMMS	25 years
Rangachary Mukundan, MPA-11	20 years
Jonathan Rau, MPA-11	20 years
Kathryn Berchtold, MPA-11	15 years
Leonardo Civale, MPA-CMMS.....	15 years
Han Htoon, MPA-CINT	15 years
Ross McDonald, MPA-CMMS	15 years
John Rowley, MPA-11	15 years
Darrick Williams, MPA-CINT	15 years
Marc Janoschek, MPA-CMMS	5 years
Cortney Kreller, MPA-11	5 years



Los Alamos researchers in collaboration with external colleagues have successfully developed and tested a high-throughput electromagnetic isotope separator (EMIS) capable of producing gram-scale quantities of high purity isotopes in a single day.

Los Alamos researchers include Chris Leibman, Jon Rau, and Kevin Dudeck (Materials Synthesis and Integrated Devices, MPA-11); Ilija Draganic and Larry Rybarcyk (Accelerators and Electrodynamics, AOT-AE); and Tyler Bronson and James Journey (Manufacturing Science and Engineering, MET-2).

Essential support contributions were made by Laboratory staff in mechanical design engineering (AOT-MDE), logistics and electrical safety (LOG-SUP, LOG-HERG, LOG-CS), and information protection (SAFE-IP).

Readiness in Technical Base and Facilities (RTBF) was responsible for procurement of the separator and the plutonium sustainment program is responsible for helping advance the source design and testing. The work supports the Laboratory's Stockpile Stewardship mission and Materials for the Future science pillar.

Technical contacts: Chris Leibman, Jon Rau

HeadsUP!

Taking action to protect the environment

LANL's Environmental Management System

The Laboratory has 12 Governing Policies for executing work, accomplishing mission, and providing management and oversight. The Governing Policy on the Environment ensures that all work is performed in a way that protects the environment.

As stewards of our environment and to achieve our mission in accordance with all applicable environmental requirements, we set continual environmental improvement objectives and targets using an Environmental Management System (EMS). An EMS is a set of processes and practices that enable an organization to protect the environment, prevent or mitigate adverse impacts, assure compliance, improve performance, communicate with interested parties, and provide management with the information needed to make effective environmental decisions. The Lab's EMS is certified to ISO 14001, which is an internationally recognized environmental management standard.

Every year, each directorate evaluates its activities and sets new environmental goals. These goals are documented in directorate-level environmental action plans. In MPA, our goals are included in the ADEPS action plan. Actions for this year include some goals from the past as well as new goals:

- Review of our chemical inventory to develop a proposal for disposal of unneeded chemicals > 10 years old with preliminary data suggesting this is one-third of all the chemicals in ADEPS;
- Identify all remaining SF₆ sources to determine if a path forward exists to either eliminate or reclaim SF₆;
- Acknowledge pollution prevention, recycling, etc., activities of employees;
- Communicate EMS information in posters, newsletters, division meetings, etc.;
- Support disposition and cleanup of legacy equipment, including the basement of TA-3 Building 34;
- Support a housekeeping day to include recycling, salvage, burn boxes, etc.;
- Support the implementation of LED lighting;
- Evaluate storm water monitoring requirements at Sigma; and
- Continue to work with the Lab's Environmental Sustainability Program Smart Lab to reduce energy usage initiative at MSL and TFF; CINT is under consideration for future work in this area.

If you have any questions concerning our EMS, please contact Dianne Wilburn, dianne@lanl.gov, EMS POC for ADEPS, or Jeff Willis, the MPA POC. More information can also be found on the Laboratory's EMS website: int.lanl.gov/environment/ems/.



Highlights of 2016: Above: at TA-3, Building 34, we completed packaging some of the equipment from the basement as low level waste. This effort is ongoing. Below: items from TA-3, Building 34 that were sent to a smelter in Texas for destruction and recycling.



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To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822 or adeps-comm@lanl.gov. To read past issues see www.lanl.gov/orgs/mpa/materialsmatter.shtml.



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